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THEORETICAL PREDICTION OF CRITICAL PYROLYSATE MASS FLUXES OF A MATERIAL TO MITIGATE SPACECRAFT OR PLANETARY HABITAT FIRE

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Future deep space exploration and plans for planetary settlements prompted researchers to address variety of challenging engineering problems. One problem is developing materials that can mitigate an event of interplanetary spacecraft fire. A numerical simulation of piloted ignition delay time of solid fuel material for PMMA sample, subjected to various incident radiant heat fluxes and airflows was developed based on thermo-chemical solid phase model. The model incorporates, conduction, convection, surface re-radiation and radiation surface absorption heat transfer modes and solid phase chemical degradation described by first order Arrhenius law chemistry. The predicted surface temperature rise adequately captured the measured surface temperatures for forced air flow velocities induced by buoyancy relevant to normal gravity environments. Based on the measured onset temperature of ignition the critical pyrolysis, fuel vapour mass flow rate was deduced in normal gravity conditions. The critical fuel vapour mass flow rate relevant to interplanetary environment was extrapolated based on normal gravity data. The results highlights the urgent need for space policy makers and stake holders to provide more funding directed towards design and fabrication of ground based facilities simulating planetary environments in order to enhance and leverage future planetary habitat designs with capabilities of mitigation on board events of fires.

Keywords: Pyrolysis, fuel vapour flow rates, Ignition delay time, planetary environment, PMMA, numerical simulation, Fire prevention

1. INTRODUCTION

Creating space settlements on planets in outer space where prevailing conditions are conducive of sustaining life is of primary interest for space policy makers and other stakeholders, this interest perhaps stems from the principle of protecting the human mankind. While it is unlikely that the human race will be subject to catastrophic events on earth such as global pandemics or a collision course with large asteroid, it is our responsibility to be prepared for those unimaginable events, in addition, expenditures directed towards advanced technologies development for space exploration will reciprocate back by raising the living standards on our planet through commercialization of those advanced technologies on earth civilian market and therefore promoting the wellbeing and comfort in our daily lives.

Based on the same principle of preserving human life on earth, creating permanent human planetary habitat will increase the probability of an event of fire and the loss of life, especially in remote planetary habitat environments where there is limited scope of rescue operations, such as on Mars. Developing materials that can retard passively an event of fire is of primary interests for engineers and habitat designers [1], the other criteria in addition to fire retardation is a material that will be able to protect astronauts from galactic solar radiation (GCR) and solar flare bursts which constitutes of high energy particles; these protons can sustain fatal human death in few minutes of human body bombardments. The above two aspects of the problem, mitigating an event of fire and reducing the dosage of radiation prompted researchers for looking into PMMA- Polymethyl methacrylate which is the subject of this paper investigation.

It was shown that the main criteria's for reducing the amount of radiation, is material with higher hydrogen content and with minimum Z/A which is the ratio of the atomic number to atomic weight, and therefore PMMA is one of the good candidates. Minimum Z/A is a first order indication of the potential to reduce secondary neutron production. In addition lower Z contributes to lesser excess of neutrons. Shielding the spacecraft with PMMA can provide sufficient reduction of radiation levels that is compatible with the long term space missions. While other traditional competitive material such as Aluminium is considered good candidate for direct radiation reduction it was found that it is primary source of secondary particle generation and therefore falls in favour as suitable insulator [2]. To that end, pursue of materials that can reduce primary and secondary particle emissions has led to both PMMA and Polyethylene [2]. Furthermore, carbon composites are within current technologies.

The ignition of solid fuel materials mainly depends on the material properties and the surrounding environmental conditions. For piloted ignition, the ignition is being assisted by source of ignition, as the solid fuel is exposed to a heat source, the surface temperature of the material starts to rise to a point where fuel vapour began to emanate from the surface, the fuel vapour mixes with the boundary layer oxidizer assuming forced convection process until a condition of lean flammability limit is attained. Beyond this point the ignition will start and depending on the environmental conditions the flame will be sustained on the surface of the solid fuel slab material [3]. It has been demonstrated that the ignition and subsequently the flame

NOMENCLATURE			
A	Frequency factor [1/s] or Atomic weight	Z	Pre-exponential factor in the Arrhenius Law [1/s] or Atomic number
C	Specific heat [J/gr K]		
E	Activation energy [J/mole]	Greek	
gr	grams	α	Fraction
Gr	Grashof number	γ	Fraction of in-depth absorption
h_{conv}	Convection coefficient [W/m^2K]	λ	Thermal conductivity
h	Enthalpy	ε	Emissivity of the sample
k	Thermal conductivity [W/mK]	ρ	Density [kg/m^3]
K	The rate of the reaction [J/°C-sec]	∞	Ambient
L	Sample thickness [cm]	σ	Stefan-boltzman constant
m	Mass [g]	Δ	Difference
\dot{m}''	Mass flux [g/m^2 -sec]	δ	Thickness of boundary layer
Nu	Nusselt number	Subscripts	
Pr	Prandtl number	v	Pyrolysate vapour
\dot{q}	External radiant heat flux [kW/m^2]	\circ	Initial or observed
$\dot{q}_{rad, in-depth}$	In-depth radiant absorption	s	initial, or sample, or solid
R	Ideal gas constant [J/mole K]	<i>surf</i>	Surface of the testing sample
Re	Reynolds number	<i>amb</i>	Ambient
Q, ΔH	Heat of combustion [kJ/gr]	r	Reference
t	time [s]	ig	Ignition
T	Temperature [K]	g	Gas
U	velocity [m/sec]	Superscripts	
X	Coordinate along the sample thickness.	\wedge	To the power

spread is a function of the material properties, the density, the thermal conductivity and the specific heat constant in addition to environmental conditions such as forced flow velocity and the ignition source. The ignition delay time of PMMA has been extensively [4, 5] studied under normal gravity environment in order to better develop material that can retard an event of fire on earth environment. The ignition delay time was being evaluated for various materials experimentally through piloted ignition test apparatus where a solid fuel slab is placed horizontally, and various forced flow velocities were generated and the piloted ignition delay time was estimated [5]. In parallel to this a numerical computational model was developed in order to validate the experimental data. The outcome of those studies showed that the onset of piloted ignition is related to the surface temperature rise of the material where beyond certain surface temperature the material ignites. Other researchers argued [6] that a more accurate analysis should be related to the fuel vapour mass flux evolving from the surface sample, and subsequently linking the lean flammability limits with the environmental conditions to sustain a flame. The lean flammability approach gained more traction, by simulating the surface temperature rise of the solid fuel material subject to an external radiation heat flux and various forced convection velocities. Once validation associated with prediction and measured solid surface temperature is achieved, the critical fuel vapour mass flux evolving from the sample is evaluated numerically. Based on the above methodology one could rank

the materials flammability and select the best material under investigation to mitigate an event of fire by estimating the asymptotic critical pyrolysate fuel vapour mass flux beyond which ignition is not achieved for a given external heat flux.

The main challenges associated with this research are to estimate the surface temperature rise and the critical fuel vapour mass flux in partial and microgravity environments. The difficulty stems from the fact that it is impossible to simulate very low magnitude forced flow velocities prevailing in interplanetary environments on earth based facilities due to limitation imposed by natural convection, and therefore, unless conducting research on space based environment facilities, progress is challenging and somehow problematic. On microgravity environments the typical magnitude of forced flow is on the order of 0.1 m/sec which is a challenging to simulate on earth based facilities. Furthermore, the research has been focused mainly on earth based facilities and on the international space station on microgravity environments; recently NASA has invested in rotation facilities and researched on solid fuel material flame spread using centrifuges were conducted to simulate partial gravity environments [7, 8]. Despite these efforts, there is great lack of research in many areas related to partial gravity environment in general and even more so on fire and combustion; while the two extremes of earth and microgravity environments are reasonably well understood the partial gravity environments such as the prevailing conditions

on Mars and the Moon are still to be explored. Furthermore, it had been demonstrated that flammability of material is enhanced in partial gravity environment [9]. Parabolic flight tests can simulate partial gravity, but those tests are limited in terms of time scales and therefore can be considered not attractive. Therefore this paper is an attempt to accelerate UK and European space stakeholders advocating to address the gap in partial gravity environment by anchoring initiatives and claims based on this research output.

2. EXPERIMENTAL APPARATUS

The numerical simulation that will be described in the following section will simulate the governing equations emulating the flow and heat transfer of the experimental apparatus [10] depicted in Fig. 1. As it is illustrated in the figure, a slab of PMMA is placed horizontally in a frame holder, the thickness of the slab can be adjusted so that the experiment can be conducted under thermal thin or thermally thick conditions. A radiant panel is placed on top of the solid sample and the radiant heat flux can be set to various magnitudes so that the sample can be exposed at different radiant heat fluxes values. The apparatus consist also of a piloted ignition source and the environmental conditions associated with forced convection can be controlled to simulate typical forced flow magnitudes prevailing on earth environment which are due to buoyancy effects. The sample is carefully prepared to embed thermocouples at different surface locations in order to measure the surface temperature rise of the sample till the point of ignition; the point of ignition will be determined by the infinite rise of the temperature of the sample. The back surface of the solid sample is insulated to prevent any heat loss and to simulate actual real life scenario conditions.

3. MODEL FORMULATION

A solid- phase model is described below [5] which consists of a mass balance equation, energy equation and a solid phase decomposition based on Arrhenius law chemistry. The mass balance is

$$\frac{\partial \rho_s}{\partial t} = -\frac{\partial \dot{m}''}{\partial x} \quad (1)$$

equation (1) implies, the mass flux \dot{m}'' accumulation is due to the change in the solid density ρ_s .

The conservation of energy is given

$$\rho_s \frac{\partial h_s}{\partial t} + \dot{m}'' \frac{\partial h_g}{\partial x} = \frac{\partial}{\partial x} \left(\lambda_s \frac{\partial T_s}{\partial x} \right) + \frac{\partial q_r}{\partial x} + (Q_s - h_s + h_g) \frac{\partial \rho_s}{\partial t} \quad (2)$$

Where h is the enthalpy defined as

$$h_i = \int_{T_\infty}^T C_i dT,$$

and the subscript can be s or g which represent solid or the gas phase. Careful examination of the energy equation shows the following; the first term is the rate of increase of enthalpy in the solid, the second term is the contribution for the heat transfer as a result of the mass flow through the solid. This term might be neglected since the amount of volatile generated until the point of ignition is small and can be ignored. Furthermore the large amount of volatile is generated near the surface. The second term on the right hand side is the in-depth absorption of radiation by the solid with $q_{r,s}$ the external radiative heat flux reaching the surface of the solid. It is reasonable to assume that the radiation is absorbed at the surface, since the absorption depth is typically very small. The last term on the right hand side is the contribution of the energy of the thermal decomposition.

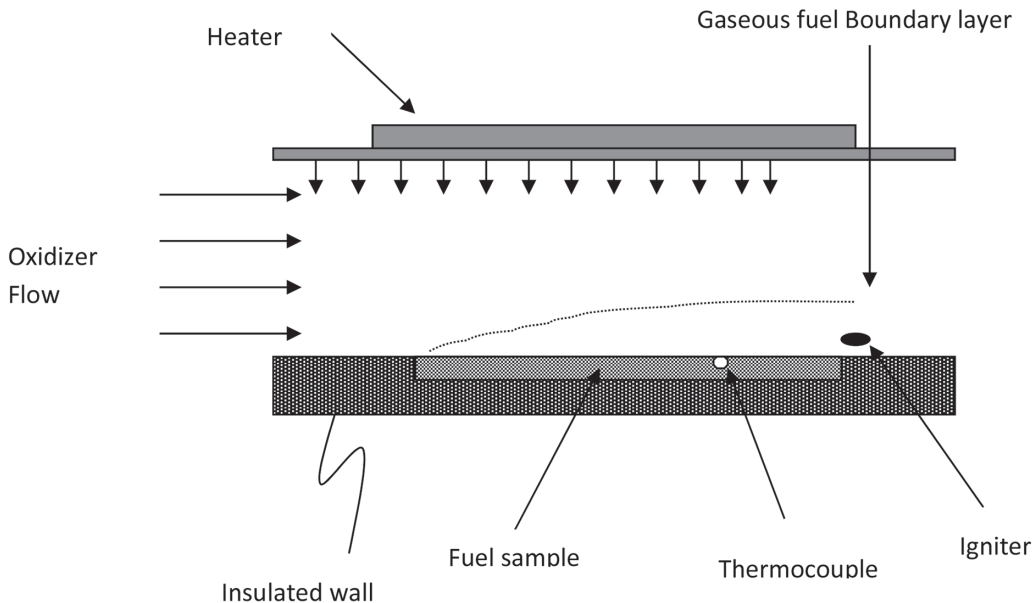
The overall kinetic equation is used to represent the decomposition equation

$$\frac{\partial \rho_s}{\partial t} = -A_s (\rho_s) \cdot \exp(-E_s / RT_s) \quad (3)$$

If we assume that the decomposition takes place at or near the surface then from (3) and (1) we get

$$\dot{m}''_s = \bar{A}_s \cdot \rho_s \cdot \exp(-E_s / RT_s) \quad (4)$$

Fig. 1 Schematic showing the experimental apparatus [10].



The initial and boundary conditions are.

$$T_s(x, 0) = T_\infty, \quad \rho_s(x, 0) = \rho_{s\infty}, \quad \dot{m}'' = 0 \quad (5)$$

$$\text{at } t = 0, \quad -l < x < 0$$

$$\lambda_s \frac{\partial T_s}{\partial x}(x=0) = -\lambda \frac{\partial T}{\partial x}(x=0) - \varepsilon \sigma (T_s^4 - T_\infty^4) \quad (6)$$

$$\text{at } x=0, \quad t > 0$$

equation (6) represents the coupling between the gas and solid phase energy equation. On the other hand if the gas phase radiation or absorption is negligible and if

$$[-\lambda(\partial T / \partial x)]_{x=0} = h_c(T_s - T_\infty) \quad (7)$$

$$-\lambda_s \frac{\partial T_s}{\partial x} = \alpha q_{rs} - h_c(T_s - T_\infty) - \varepsilon \sigma (T_s^4 - T_\infty^4) - \dot{m}''_s \cdot Q_{net}$$

$$\text{at } t > 0, \quad x = -l \quad (8)$$

two boundary conditions are possible, this depends on the thickness of the solid, for thermally thick, then $T_s(l \rightarrow \infty, t) = T_\infty$, on the other hand for thermally thin, a back boundary condition should be applied [11].

The above model has certain assumption built into it to make the problem simplified and tractable. Those assumptions are no motion inside the solid, such as bubbles, the sample is exposed by a uniform radiant heat flux, the characteristic length of the sample is much larger than the thickness of the sample. This assumption is concerned with the validity of one dimensional analysis, the volatiles are leaving the sample almost instantly as they are being generated, First order Arrhenius law is used to model the decomposition of PMMA, the kinetic parameters are extracted from TG/DTA available in the public domain and thermal equilibrium exists between the PMMA sample and the volatile being generated. The above generic model and the boundary conditions can be simplified for the PMMA sample and the resulting formulation is

$$\frac{\partial \rho}{\partial t} = \frac{\partial m_v}{\partial x} \quad (9)$$

$$\frac{\partial(\rho h)}{\partial t} - \frac{\partial(m_v h_v)}{\partial x} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + Q \frac{\partial \rho}{\partial t} + q_{rad, in-depth} \quad (10)$$

$$\frac{\partial \rho}{\partial t} = -z \rho \exp\left(-\frac{E}{RT}\right) \quad (11)$$

where

$$h = \int_0^T C_p dT \quad \text{the enthalpy for PMMA}$$

$$h_v = \int_0^T C_v dT \quad \text{for the fuel vapour}$$

and the boundary conditions are

$$T = T_\infty, \quad \rho = \rho_0, \quad m_v = 0 \quad \text{at } t = 0$$

$$\varepsilon q_{rad} = -k \frac{\partial T}{\partial x} + h_{conv}(T_{surf} - T_{amb}) + \varepsilon \sigma T_{surf}^4 \quad \text{at } x = 0$$

$$\frac{\partial m_v}{\partial x} = 0 \quad \frac{\partial T}{\partial x} = 0 \quad \text{at } x = L$$

$q_{rad, in-depth} = \varepsilon q''_{rad}$, where q''_{rad} is the incident heat flux on the PMMA sample. The specific heat for the fuel vapour is assumed to be of that of air, and the specific heat for the PMMA was selected as $C_p = 1.5 [J/grK]$ and $C_p = 2.0 [J/grK]$ for the range below the glass transition temperature and above the glass transition temperature respectively [12] and the PMMA material heat capacity was selected based on reference [13]. The thermal properties of PMMA are shown in Table 1.

TABLE 1: Thermal Properties of PMMA [12, 13, 18, 19].

Property	Unit	Material : PMMA
ρ	kg/m ³	1200
k	W/mK	0.2
C	J/grK	1.5
Z	1/s	2.02E14
E	J/mol	1.42E5
Q	kJ/gr	-26.64

In order to calculate the convective heat transfer coefficient [6] for vertical plate orientation

$$h_{conv} = k_{air} Nu_{total} / L_{flow}$$

the correlation

$$Nu_{total}^3 = Nu_{forced}^3 + Nu_{buoyant}^3$$

where

$$Nu_{forced} = 0.664 Re^{1/2} Pr^{1/3}$$

and

$$Nu_{buoyant} = \frac{4}{3} \left(\frac{Gr}{4} \right)^{1/4} G(Pr)$$

respectively. The values for the horizontal plate are calculated and the effect of buoyancy is neglected. The values of h_{conv} are 2.33, 2.86, 6.7 and 9.5 W/m²K for airflow of 0.09, 0.15, 1.0 and 1.75 respectively. For a thin sample the heat transfer from the back of the sample to sample holder need to be considered, thus this is incorporated in the boundary condition. The low airflow of the order of 0.1 m/s was chosen in order to simulate conditions in the international space station associated with heating and ventilation systems.

The governing equations and the boundary conditions combined are a set of nonlinear parabolic system of equations; the Crank-Nicolson discretization scheme is utilized to solve the system of equations.

4. RESULTS AND DISCUSSION

The predicted, based on numerical simulation and measurement,

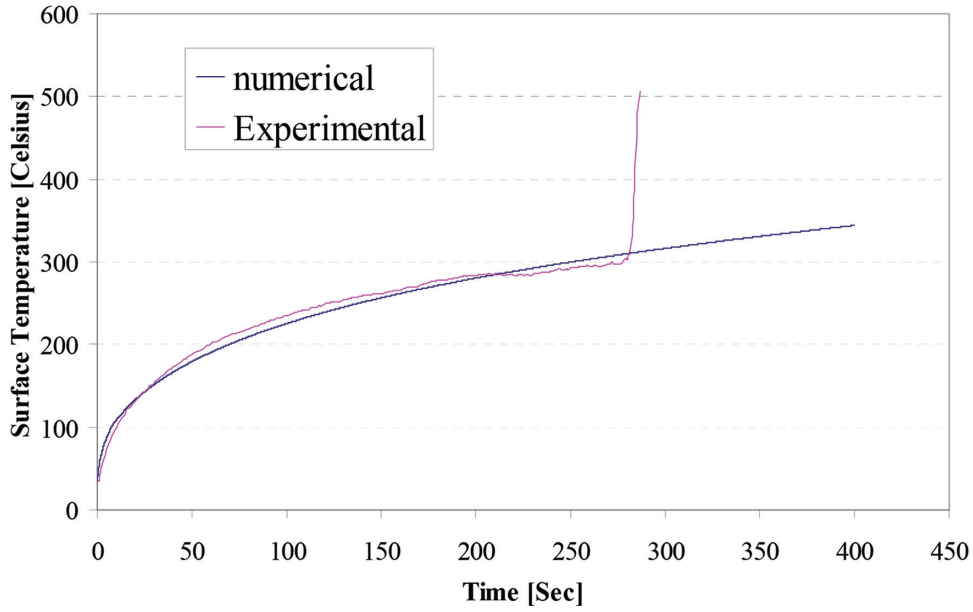


Fig. 2 Predicted and measured surface temperature for industrial-grade PMMA for airflow velocity of 1.75m/sec and external heat flux of 16.5kW/m².

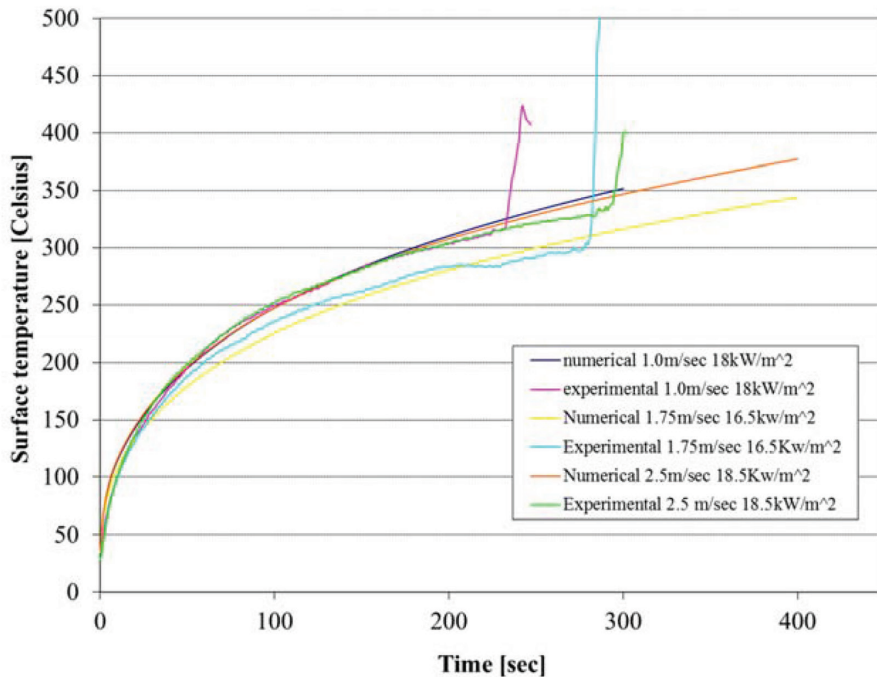
surface temperature of PMMA at airflow of 1.75 m/sec and at incident heat flux of 16.5 W/m² is shown in Fig 2. The curves illustrate that the numerical simulation captured the measured [14] temperature surface rise of the PMMA sample. The infinite temperature rise of the experimental curve [14] demonstrates the point of ignition and the onset ignition occurs at around 279 seconds after the sample is impulsively exposed to the incident radiant heat flux.

Figure 3 illustrates the predicted and measured surface temperature at various airflows of 1.0, 1.75 and 2.5m/sec and at incident heat fluxes of 18, 16.5 and 18.5 W/m² respectively. The results further corroborate the observation that the numerical simulation matches the experimental surface [14] temperature

rise and indicates the onset of ignition occurs after 230, 279 and 300 seconds respectively. The results illustrate that the ignition delay time on normal gravity conditions increases as the magnitude of the oxidizer airflow increases which is attributed to higher convection which results in more time required to attain the lean flammability conditions to sustain an ignition.

Figure 4 illustrate the critical predicted pyrolysate mass flow rates for oxidizer airflows of 1.0, 1.75 and 2.5 m/sec and the corresponding incident heat fluxes of 18, 16.5 and 18.5 W/m². The values depicted in the figure illustrate that for higher forced velocities induced by buoyancy in normal gravity conditions, the predicted critical pyrolysate mass flow rates to attain ignition is higher. The numerical range of vapour fuel flow rates values

Fig. 3 Predicted and measured surface temperature for PMMA at different airflow velocity and heat fluxes.



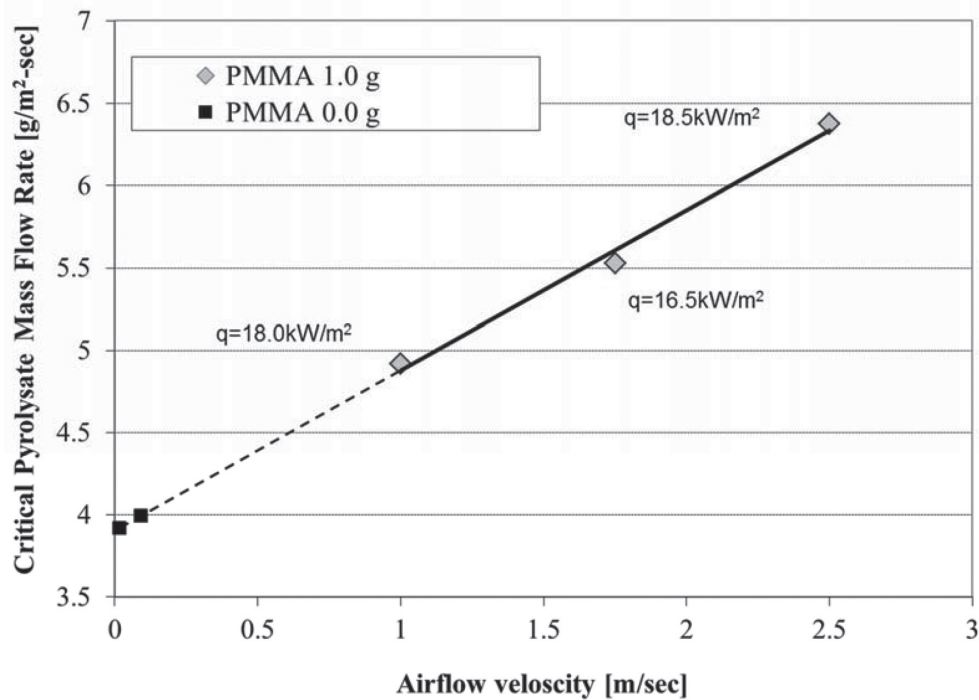


Fig. 4 Predicted critical mass fluxes for various airflow velocities and heat fluxes.

relevant to normal gravity conditions reported in this study compared favourably with fuel vapour mass flow rates reported elsewhere [15, 16, 17]. Furthermore, based on pyrolysate mass fluxes values corresponding to 18, 16.5 and 18.5 W/m² an approximate linear correlation can be developed as depicted by the dash line to extend the range of the oxidizer airflow down to value of 0.09 and 0.15 m/sec which are values relevant for interplanetary conditions. Based on extrapolation of vapour fuel mass fluxes in normal gravity the values depicted in Figure 4 are 3.92 and 3.99 g/m²-sec in 0.0g gravity. It is worth noting, since current ground based facilities simulating interplanetary environments, such as parabolic flights have challenges and limitations as microgravity and partial gravity periods are limited to freefall dive periods of the aircraft, of around 20 seconds duration, this implies that in order to conduct such experiments on board the aircraft an incident heat fluxes of higher than 30 W/m² are required in order for piloted ignition to occur within controlled time frame of steep dives. In addition parabolic flights suffer from g-gitter which will require careful experimental procedures and further data processing treatments. Other ground based facilities such as drop tower experiments also have very limited time durations.

5. CONCLUSIONS AND FUTURE RECOMMENDATIONS

Numerical simulation of ignition delay time of solid fuel

material of PMMA sample subjected to various incident radiant heat fluxes and oxidizer airflow was developed based on thermo-chemical solid phase model. The model incorporates conduction, convection, surface re-radiation and radiation surface absorption heat transfer modes and chemical degradation described by first order Arrhenius law chemistry. The predicted surface temperature rise adequately captured the measured surface temperatures for forced air flow velocities induced by buoyancy relevant to normal gravity environments. Based on the measured onset temperature of ignition the critical pyrolysate fuel vapour mass flow rate was deduced in normal gravity conditions. The critical fuel vapour mass flow rate relevant to interplanetary environments was extrapolated. The results can be further corroborated by conducting ground based planetary environment testing, this highlights the urgent need for space policy makers and stake holders to provide more funding directed to the design and fabrication of ground based facilities simulating planetary environments in order to enhance and leverage future planetary habitat designs with capabilities of mitigation on board events of fires.

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The author, Dr. Sam M. Dakka developed the piloted ignition simulation program using open source FORTRAN software. The research was performed with no funding support.

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